Introduction to STAN

A probabilistic programming language

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Content[1]

An introduction to STAN, a well-designed and easily used tool, for statistical modeling.

- What is STAN.
- How STAN works.
- How to write a STAN script.
- How to run it and analyze the result.

[1] https://github.com/beyondpie/intro_to_stan

Section 1

The big picture

What is STAN [2]

- A *programming language*
  - It supports array data structure, while loops, and conditionals.
  - The syntax much like C++. But no need to worry about C++.
  - STAN itself is written in C++.
  - A model written in STAN needs to be compiled.
- Specifically designed for the *statistical modeling*
  - Vector, matrix and their operations
  - A series of probabilistic functions
  - A series of blocks to describe a statistical model.
  - Support sampling, maximum likelihood estimation and variational inference.

[2] https://mc-stan.org

STAN script

```
// A typical stan script is composed by several modules/blocks.
functions {}
data {
  int N;
  real y[N];
  real<lower=0> sigma_y
}
transformed data {}
parameters {real mu;}
transformed parameters {}
model {
  mu ~ normal(0.0, 1.0);
  for (n in 1:N) { y[n] ~ normal(mu, sigma_y);}
}
generated quantities {
  // unused in the model
  // generate replicated data or monitor convergence
  real square_mu;
  square_mu = mu * mu; }
```

Section 2

Behind STAN

MCMC Sampling in STAN

- *Hamiltonian Monte Carlo (HMC)* provides a general sampling procedure for Bayesian inference: using the derivatives of the density function.
- HMC and its adaptive variant the no-U-turn sampler (NUTS) [Hoffman and Gelman, 2014] are used in STAN. NUTS is the default one.
- You DON'T need to write the derivatives in STAN.

HMC in STAN

- Sampling goal: $p(\theta|y)$, the posterior distribution given data y.
- HMC introduces auxiliary momentum variables ρ. $p(\rho, \theta) = p(\rho|\theta)p(\theta)$. In STAN, $p(\rho|\theta) \sim \mathcal{N}(0, M)$, is independent of θ
- Parameters in HMC [See Chapter 15 in STAN Reference Manual]
    - The discretization time ϵ [3] will be automatically optimized during warmup to match an acceptance rate parameter δ (default is 0.8). Increasing δ will force the sampler to use small step sizes, and increase the effective sample size per iteration.
    - The M^{-1} (default a diagonal matrix) is estimated during warmup[4].
    - Number of steps taken L is dynamically adapted during sampling (and during warmup) in NUTS, which is controlled by a predefined parameter *treedepth*.

[3] STAN also allows step-size jitter, which means "jittered" randomly during sampling to avoid poor interactions. Default is 0, producing no jitter.

[4] STAN supports *Euclidean HMC*. M could be configured by the user.

Bounded parameters transformation

Besides auto-tuning the parameters in HMC (NUTS), STAN will transform the bounded variables to an unconstrained ones in the backend.

The basis idea is to set a one-to-one transformation $y = f(x)$:

$$p_Y(y) = p_X(f^{-1}(y))|detJ_{f^{-1}}(y)|$$

Transformations: examples

- $y = \log(x - a)$ if x has lower bound a.
- $y = logit(x) = \log \frac{x}{1-x}$ if $x \in (0, 1)$.
- $y = logit(\frac{x-a}{b-a})$ if $x \in (a, b)$.
- If x is ordered, then $y_k = \log(x_k - x_{k-1})$.
- If $x_k > 0, \sum_k^K x_k = 1$, then
  $y_k = logit(z_k) - log(\frac{1}{K-k}); z_k = \frac{x_k}{1-\sum_{s=1}^{k-1} x_s}, z \in \mathcal{R}^{K-1}$.
- When x is a correlation matrix, find the upper triangular w such that $x = ww^T$, which can be done Cholesky decomposion. Then an inverted transformation is designed on w [See chapter 10 in STAN Referenc Manual for details].

STAN Math Library

- STAN owns a mathematical library [Carpenter et al., 2015] named STAN Math Library that can automatically get the gradients (not the numerical approximation) and support matrix operations ,linear algebra, most common probability functions and so on.
- It's a C++, reverse-mode automatic differentiation library. Not limited to STAN, and designed to be extensive, efficient, scalable and so on.

Reverse-Mode Automatic Differentiation: an example

$f(y, \mu, \sigma) = -\frac{1}{2}(\frac{y-\mu}{\sigma})^2 - \log \sigma - \frac{1}{2} \log 2\pi$

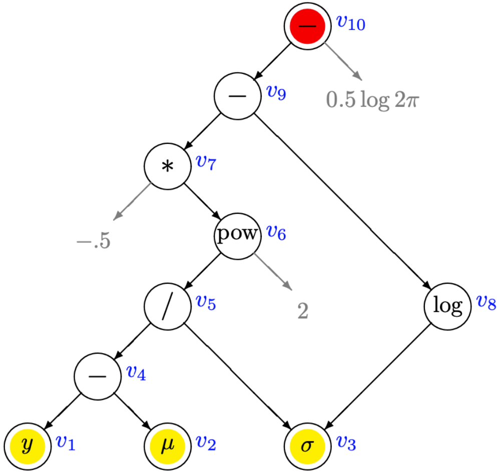


Figure 1: Expression graph of the normal log densityfunction (carpenter2015stan)

Section 3

RUN STAN

How to use STAN with R?

STAN development team provides lots of choices for R users.

- **RStan**: the R interface to STAN.
  - One can fit the model in R and access the output. It relies on Rcpp to call C++ code, and hard to keep updates with the newest STAN.
- **CmdStan**: command-line / shell interface.
  - One can control the compiling easily, e.g., add multi-thread support and GPU support. It directly uses the latest STAN, but not flexible.
- **CmdStanR**: a lightweight interface to CmdStan. You can control CmdStan without leaving R.
- **brms**[Bürkner, 2016]: will make the STAN script for you and pass it to **RStan**.
- rstanarm
  - Bayesian applied regression modeling (arm) via rstan. You can use the customary R modeling sytax, like *glm* with a *formula* and *data.frame*.

Show me an example

Let's consider a simple example.

- Suppose we have N binary observations $y_1, y_2, \ldots, y_N$. They are the *i.i.d* samples from a $Bernoulli$ distribution under the parameter θ.
- Our goal is to infer θ.

Set up the STAN env in R.

```
library(cmdstanr)
# Note: the cmdstan home path is from my computer.
set_cmdstan_path(path = paste(Sys.getenv("HOME"),
                 "softwares",
                 "cmdstan-2.23.0", sep = "/"))
library(bayesplot)
library(posterior)

cmdstan_path()
[1] "/Users/beyondpie/softwares/cmdstan-2.23.0"
cmdstan_version()
[1] "2.23.0"
```

STAN script

```
bern_mod <- cmdstan_model("bernoulli.stan",
                          ## STAN need to be complied.
                          compile = TRUE)
## show the content in the stan script.
bern_mod$print()
data {
  int<lower=0> N;
  int<lower=0,upper=1> y[N];
}
parameters {
  real<lower=0,upper=1> theta;
}
model {
    // uniform prior on interval 0, 1
  theta ~ beta(1,1);
  y ~ bernoulli(theta);
}
```

Let's feed it some data I

```r
bern_data  <- list(N = 10, y = c(0,1,0,0,0,0,0,0,0,1))
## Run MCMC using the 'sample' method
bern_mcmc <- bern_mod$sample(data = bern_data,
                              seed = 355113,
                              chains = 4,
                              parallel_chains = 2,
                              show_message = FALSE)
```

Summary of the sampling in STAN

```r
## use `posterior` package
bern_mcmc$summary("theta", "mean", "sd" , "rhat",
                  "ess_bulk")
```

variable	mean	sd	rhat	ess_bulk
theta	0.2523255	0.1232632	1.001693	1425.133

Posterior draws I

```
draws <- bern_mcmc$draws()
str(draws)
 'draws_array' num [1:1000, 1:4, 1:2] -6.75 -6.97 -7.04 -7.15 -6.87
 - attr(*, "dimnames")=List of 3
  ..$ iteration: chr [1:1000] "1" "2" "3" "4" ...
  ..$ chain    : chr [1:4] "1" "2" "3" "4"
  ..$ variable : chr [1:2] "lp__" "theta"
## use posterior::as_draws_df to transorm the results
## into data.frame.
```

How about variational inference?

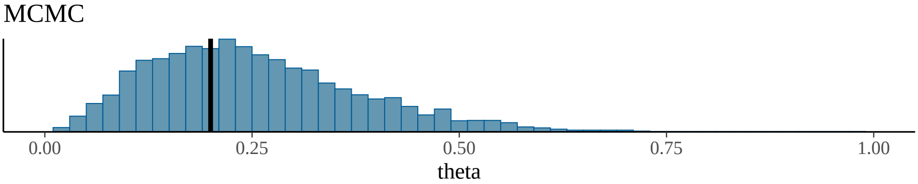
```
bern_vb <- bern_mod$variational(data = bern_data,
                                 seed = 355113,
                                 output_samples = 4000)
```

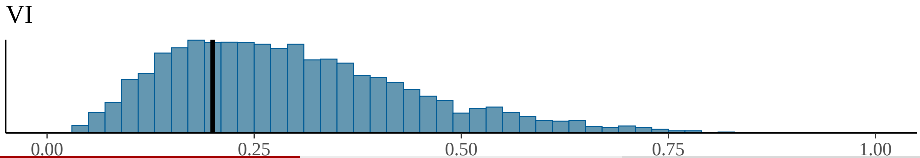
How about MLE estimation?

```
bern_mle <- bern_mod$optimize(data = bern_data,
                              seed = 355113)
```

Result Summary

```
bayesplot_grid(
  mcmc_hist(bern_mcmc$draws("theta"), binwidth = 0.02) +
  vline_at(bern_mle$mle(), size = 1.2),
  mcmc_hist(bern_vb$draws("theta"), binwidth = 0.02) +
  vline_at(bern_mle$mle(), size = 1.2),
  titles = c("MCMC", "VI"),
  xlim = c(0,1))
```





Section 4

Materials and Summary

STAN Materials

- STAN Functions
  - Use this as the reference materials. When you want some functions, just search it.
- The STAN Language Sytanx
  - You can scan this if you want to know the whole picture of STAN syntax.
- The User Guide
  - After the introduction, you could read this document smoothly.
  - Lots of examples cover different statistical modelings.
  - It could be a good material to learn statistical models.

Summary

- STAN is designed as a statistical programming language.
  - Rich of elements, such as matrix operations, probabilistic functions.
  - The clear structures of the blocks for describing a model.
  - Efficiency: C++ backend, multi-thread support, GPU support and map-reduce support.
- STAN provides a general and solid inference framework.
  - Uses *NUTS* and *HMC* for sampling.
  - Uses *ADVI* for variational inference.
  - Use *L-BFGS* for optimization, such as MLE estimation.
- STAN has lots of APIs in both R and Python. For R,
  - *cmdstanr*, *cmdstan* for compiling and run the latest STAN.
  - *bayesplot*, *posterior* for analyzing and visualizing the results.
  - *rstan* as a united interface but not support the latest STAN.
  - *brms* and *rstanamrs* simplify the process of writing STAN scripts.

Thanks!

- You can find this presentation at https://github.com/beyondpie/intro_to_stan.
- Any suggestions or Pull Requests are welcome.

Paul-Christian Bürkner. brms: An r package for bayesian generalized linear mixed models using stan. *J Stat Softw*, 2016.

Bob Carpenter, Matthew D Hoffman, Marcus Brubaker, Daniel Lee, Peter Li, and Michael Betancourt. The stan math library: Reverse-mode automatic differentiation in c++. *arXiv preprint arXiv:1509.07164*, 2015.

Matthew D Hoffman and Andrew Gelman. The no-u-turn sampler: adaptively setting path lengths in hamiltonian monte carlo. *J. Mach. Learn. Res.*, 15(1): 1593–1623, 2014.